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The Strong Interaction at Neutron-Rich Extremes

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In our JUROPA/JURECA project, we have applied powerful many-body methods to strongly interacting nuclear systems. We have developed quantum Monte Carlo calculations with chiral effective field theory interactions to study light nuclei and neutron matter. Moreover, we have systematically implemented chiral three-nucleon forces in many-body calculations of medium-mass nuclei, using renormalisation group methods in momentum space and in-medium for calculations of valence-shell interactions. This enabled us to make predictions of exotic nuclei studied at rare isotope beam facilities and of extreme neutron-rich matter in astrophysics.

1 Introduction

The microscopic understanding of atomic nuclei and of high-density matter is a very challenging task. Powerful many-body simulations are required to connect the observations made in the laboratory to the underlying strong interactions between neutrons and protons, which govern the properties of nuclei and of strongly interacting matter in the universe. Renewed interest in the physics of nuclei is driven by discoveries at rare isotope beam facilities worldwide, which open the way to new regions of exotic, neutron-rich nuclei, and by astrophysical observations and simulations of neutron stars and supernovae, which require controlled constraints on the equation of state of high-density matter. Fig. 1 shows the substantial region of exotic nuclei that will be explored at the future FAIR facility in Darmstadt.

The nuclear many-body problem involves two major challenges. The first one concerns the derivation of the strong interaction between nucleons, which is the starting point of few- and many-body *ab initio* calculations. Since nucleons are not elementary particles, but composed of quarks and gluons, the strong interaction has a very complex structure. Although it is becoming possible to study systems of few nucleons directly based on quarks and gluons[1], the fundamental degrees of freedom of quantum chromodynamics (QCD), high-precision calculations of nuclei based on quarks and gluons will not be feasible in the foreseeable future. As a systematic approach, chiral effective field theory (EFT) allows to derive nuclear forces in terms of low-energy degrees of freedom, nucleons and pions, based on the symmetries of QCD[2]. The chiral EFT framework provides a systematically improvable Hamiltonian and explains the hierarchy of two-, three-, and higher-body forces. The presence of such many-body forces is an immediate consequence of strong interactions[3].

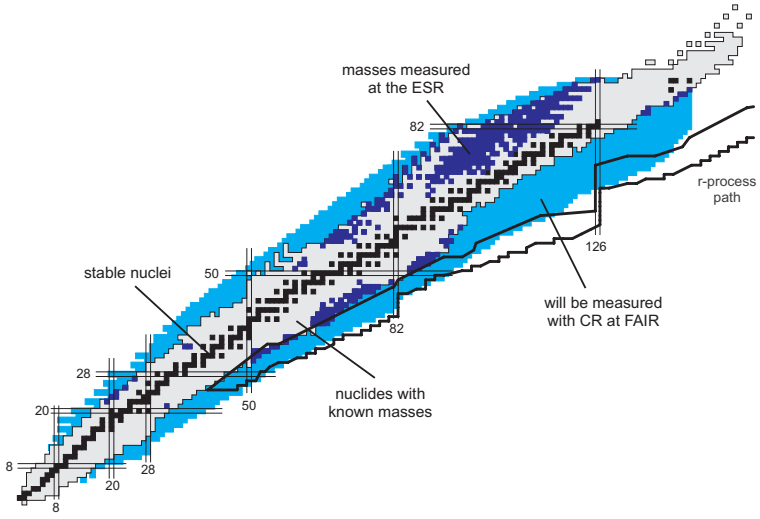

Figure 1. Chart of atomic nuclei. The black points mark the stable nuclei, while the grey region denotes all nuclei known to date. Of the latter, the points in purple have been studied with mass measurements at the GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt. The blue points mark the exotic nuclei that will be explored at the future FAIR facility. Figure courtesy Y. Litvinov (GSI).

In particular, the computation and inclusion of three-nucleon (3N) forces in many-body calculations is one of the current frontiers[4].

The second challenge concerns the practical solution of the many-body problem based on nuclear forces. Since the computational complexity grows significantly with the number of particles, up to about 10 years ago the scope of *ab initio* calculations was limited to light nuclei up to around carbon (with nucleon number $A = 12$). Due to advances on several fronts and also due to rapidly increasing computing power, this limitation has nowadays been pushed to much heavier systems (see, e.g., the recent work of Ref. 5). One key step was the development of powerful renormalisation group (RG) methods that allow to systematically change the resolution scale of nuclear forces[6,7]. Such RG transformations lead to less correlated wave functions at low resolution and the many-body problem becomes more perturbative and tractable.

Our work focuses on the derivation of RG evolved interactions and electroweak operators, the inclusion of chiral 3N forces in many-body calculations of extreme neutron-rich nuclei, and on the development of quantum Monte Carlo simulations with chiral EFT interactions, which open up nonperturbative benchmarks for nuclei and high-density matter. These calculations enable us to explore the formation of structure in exotic nuclei, the properties of neutron-rich nuclei and matter that play a key role in the synthesis of heavy elements in the universe, as well as the nuclear physics involved in applications to fundamental symmetries, e.g., for the nuclear matrix elements of neutrinoless double-beta decay that probes the nature and mass scale of the neutrinos.

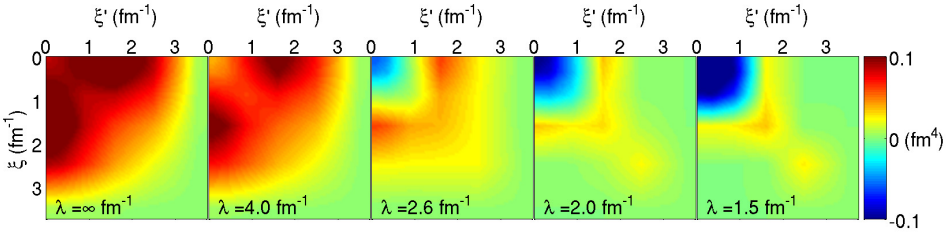

Figure 2. Contour plots of SRG-evolved 3N interactions as a function of three-body hypermomenta (see Ref. 8 for details). Shown is the systematic decoupling of low- and high-momentum parts in the interaction as the SRG resolution scale λ is lowered from left to right. (Figure taken from Ref. 8).

2 Renormalisation Group Evolution of Nuclear Interactions

The convergence behaviour and the required computational resources of many-body calculations for a given nucleus are governed by the properties of the employed nuclear forces. It is convenient to visualise nuclear interactions as a function in momentum space, where low momenta correspond to large interparticle distances and high momenta to short-range correlations. In general, a strong coupling of low- and high-momentum parts in nuclear interactions induce strong virtual excitations of particles and imply a poor perturbative convergence and large required basis spaces for the solution of the many-body Schrödinger equation. The similarity renormalisation group (SRG) allows to systematically decouple low-momentum physics from high-momentum details via a continuous sequence of unitary transformations that suppress off-diagonal matrix elements, driving the Hamiltonian towards a band-diagonal form[7]. This decoupling is illustrated in Fig. 2 on the basis of a representative chiral 3N interaction.

Computationally, the SRG evolution of two-nucleon (NN) interactions is straightforward and can be performed on a local computer. However, when evolving nuclear interactions to lower resolution, it is inevitable that higher-body interactions are induced even if initially absent. This might be considered unnatural, if nuclei could be accurately calculated based on only NN interactions. However, chiral EFT reveals the natural scale and hierarchy of many-body forces, which dictates their inclusion in calculations of nuclei and nuclear matter. In fact, the importance of 3N interactions has been demonstrated in many different calculations[3,4]. The RG evolution of 3N forces is computationally challenging since typical dimensions of interaction matrices in a momentum-space partial-wave representation can reach about $10^4 - 10^5$. This means that the required memory for storing a single interaction matrix in double precision can reach about 40 GB. For the solution of the RG flow equations it is necessary to evaluate efficiently matrix products of this dimension. Since numerical solvers of differential equations need several copies of the solution vector for a stable and efficient evolution, a distributed storage of all matrices and vectors is mandatory. For an efficient evaluation of large matrix products we have employed a hybrid OpenMP/MPI strategy for our implementation.

3 Three-Nucleon Forces and Neutron-Rich Nuclei

Nuclei with a certain number of protons and neutrons are observed to be particularly well-bound. These closed-shell or "magic" nuclei form the basis of the nuclear shell model, which is a key computational method in nuclear physics. Exploring the formation of shell structure and how these magic configurations evolve with nucleon number towards the limits of the nuclear chart is a frontier in the physics of nuclei, and the microscopic understanding from nuclear forces represents a major challenge. The theoretical shortcomings in predicting shell structure are particularly evident in the calcium isotopes. While microscopic calculations with well-established NN forces reproduce the standard magic numbers $N = 2, 8, 20$, they do not predict ^{48}Ca as a doubly-magic nucleus when neutrons are added to ^{40}Ca, see Ref. 4. As a result, phenomenological forces have been adjusted to render ^{48}Ca doubly magic, and it has been argued that the need for these phenomenological adjustments may be largely due to neglected 3N forces. In recent works[9,10], we have shown that 3N forces play a decisive role in medium-mass nuclei and are crucial for the magic number $N = 28$. For the calcium isotopes, the predicted behaviour of the two-neutron separation energy S_{2n} up to ^{54}Ca is in remarkable agreement with precision mass measurements at TITAN/TRIUMF[11] and of the ISOLTRAP collaboration at ISOLDE/CERN using a new multi-reflection time-of-flight mass spectrometer, as shown in Fig. 3. The new ^{53,54}Ca masses are in excellent agreement with our NN+3N predictions and establish $N = 32$ as a shell closure. This work was published with the ISOLTRAP collaboration in Nature[12]. The same valence-shell interactions have been successfully applied to study the spectroscopy of calcium isotopes and their electromagnetic moments.

Very recently we studied ground- and excited-state properties of all sd-shell nuclei with neutron and proton numbers $8 \leqslant N, Z \leqslant 20$, based on a set of low-resolution NN+3N interactions that predict realistic saturation properties of nuclear matter[15]. We focused on estimating the theoretical uncertainties due to variation of the resolution scale, the low-energy couplings, as well as from the many-body method. In Fig. 4 we compare theoretical and experimental two-neutron separation energies S_{2n} for all isotopic chains from oxygen to calcium ($Z = 8 - 20$). The theoretical calculations describe the overall experimental trends well, but in general our uncertainty bands underestimate the empirical values. The dominant uncertainties arise from the different Hamiltonians, with smaller differences between second- and third-order MBPT results. Typically the uncertainty range for S_{2n} is $\sim$5 MeV. The exception are $N < Z$ isotopes, more visible in heavier elements, where the differences between second- and third-order results is comparable to the uncertainty between input Hamiltonians adding up to a total uncertainty of $\sim$ 10 MeV.

Since it is not possible to solve the many-body problem exactly for general medium-mass nuclei, valence-space methods utilise a factorisation of nuclei into a core and valence nucleons that occupy a truncated single-particle space above the core. The interactions of particles in this valence-space are computed microscopically in many-body perturbation theory (MBPT), whereas the primary computation lies in the self-consistent evaluation of a large number of one- and two-body diagrams. The resulting effective Hamiltonian can then be diagonalised exactly, and within certain limits reproduces the exact eigenvalues. Very recently, we have achieved the first nonperturbative derivation of valence-space Hamiltonians using the in-medium SRG, with excellent results for the spectra of oxygen isotopes[17]. This enables a first *ab initio* connection of nuclear forces to the shell model.

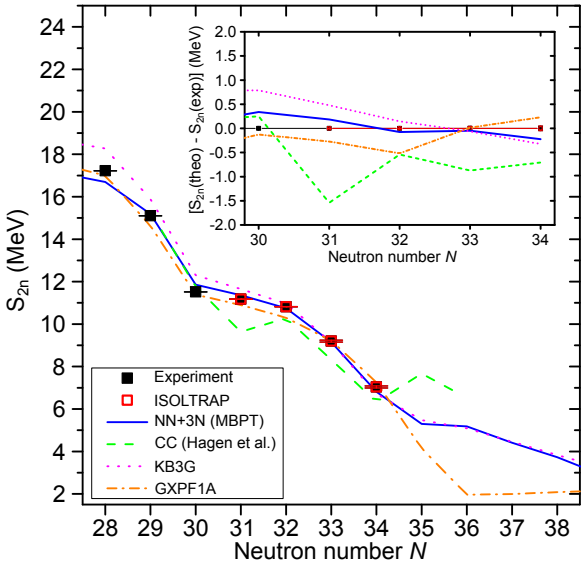

Figure 3. Two-neutron separation energy S_{2n} of the neutron-rich calcium isotopes as a function of neutron number N (see Ref. 12 for details). Shown are the new experimental results from the ISOLTRAP collaboration (red squares) in comparison with our predictions based on chiral NN+3N interactions (blue line), as well as shell-model (KB3G and GXPF1A) and coupled cluster (CC) calculations. (Figure taken from Ref. 12).

4 Quantum Monte Carlo Simulations with Chiral EFT Interactions

Quantum Monte Carlo (QMC) methods have been proven to be a very powerful tool for studying light nuclei and neutron matter[18]. In Refs. 19–21, we have presented first QMC calculations based on chiral NN interactions. This was not possible before due to nonlocalities in chiral EFT interactions. However, it is possible to remove all sources of nonlocality in nuclear forces up to next-to-next-to-leading order (N^2LO) in the chiral expansion. This enables us to perform auxiliary-field diffusion Monte Carlo (AFDMC) calculations for the neutron matter equation of state up to nuclear saturation density based on local leading-order (LO), next-to-leading order (NLO), and N^2LO NN interactions, as shown in Fig. 5. Our results exhibit a systematic order-by-order convergence in chiral EFT and provide nonperturbative benchmarks with theoretical uncertainties. For the softer interactions, perturbative MBPT calculations are in excellent agreement with the AFDMC results, as shown in Fig. 6.

These advances also opened up first Greens Function Monte Carlo calculations of light nuclei based on chiral NN interactions[21]. Recently, we implemented the leading 3N forces in QMC simulations of neutron matter and light nuclei[22,23]. This paves the way for QMC calculations with systematic chiral EFT interactions for nuclei and nuclear matter, for testing the perturbativeness of different orders, and also allows for matching to lattice QCD results in a finite volume.

The QMC methods we use in our calculations treat the Schrödinger equation as a diffusion equation in imaginary time and project out the ground-state wave function from a

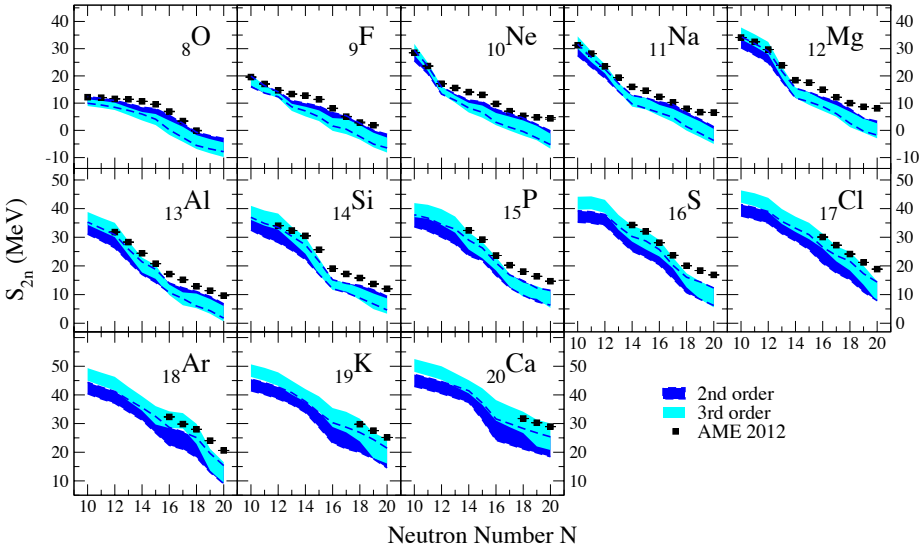

Figure 4. Uncertainty estimates for the two-neutron separation energies S_{2n} of sd-shell isotopic chains at second (blue, darker band) and third order (cyan, lighter band) in MBPT (see Ref. 15 for details) and compared to the Atomic Mass Evaluation (AME 2012)[16]. (Figure taken from Ref. 15).

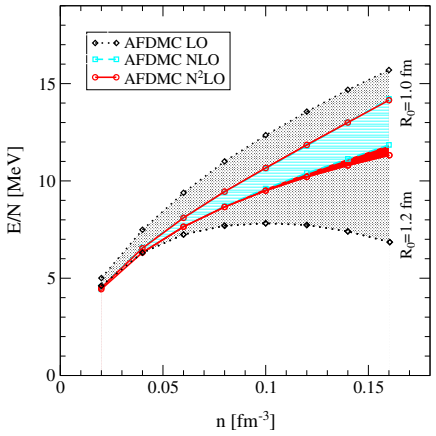

Figure 5. Neutron matter energy per particle E/N as a function of density n using AFDMC with the local chiral NN potentials at LO, NLO, and N^{2}LO. The bands are obtained by varying the cutoff $R_0 = 1.0 - 1.2$ fm and the SFR cutoff $\tilde{\Lambda} = 1000 - 1400$ MeV.

trial wave function by evolving to large imaginary times. GFMC performs, in addition to a stochastic integration over the particle coordinates, explicit summations in spin-isospin space, and is thus very accurate but computationally very costly, so that one can only access particle numbers with $A \leqslant 12$. In contrast, AFDMC also stochastically evaluates summations in spin-isospin space and shows a better scaling behaviour at the cost of less

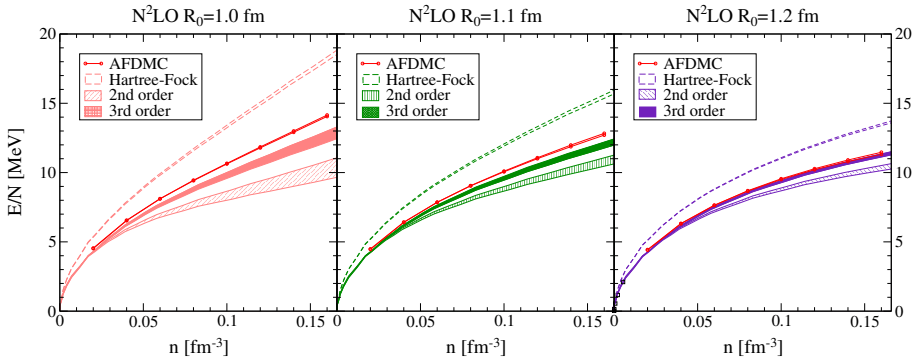

Figure 6. Neutron matter energy per particle E/N as a function of density n based on AFDMC and MBPT calculations (see Ref. 20 for details). The different panels show results using local N^{2}LO NN interactions with different resolution scale $R_0 = 1.0 - 1.2$ fm (the latter being the softest interaction). For the MBPT results, we show the Hartree-Fock energies as well as the energy at second and third order. The width of the bands provide a measure of the theoretical uncertainty. For the softer interactions (right panel), the perturbative calculations are in excellent agreement with the AFDMC results. (Figure taken from Ref. 20).

accuracy. We can thus simulate 66 fermions in our neutron matter calculations. For our QMC simulations we typically average over $5 - 10$k walkers for several thousand time steps. Since we use independent walkers, the code is easily parallelisable and shows an excellent and almost linear scaling behaviour with the number of cores. Typically, we use $200 - 400$ cores. In contrast to SRG transformations, we have only moderate memory requirements of typically 1 GB per core.

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